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Local Environment Distribution in Ab Initio Liquid Water[1]
BISWAJIT SANTRA, ROBERT A. DISTASIO, JR., ROBERTO CAR, Department of Chemistry, Princeton University, Princeton, NJ 08544, USA — We have analyzed the distribution of local environments in liquid water at ambient conditions and its inherent potential energy surface (IPES) based on state-of-the-art *ab initio* molecular dynamics simulations performed on 128 molecules implementing hybrid PBE0 exchange [PRB **79**, 085102 (2009)] and van der Waals (vdW) interactions [PRL **102**, 073005 (2009)]. The local environments of molecules are characterized in terms of the local structure index (LSI) [JCP **104**, 7671 (1996)] which is able to distinguish high- and low-density molecular environments. In agreement with simulations based on model potentials, we find that the distribution of LSI is unimodal at ambient conditions and bimodal in the IPES, consistent with the existence of polymorphism in amorphous phases of water. At ambient conditions spatial LSI fluctuations extend up to $\sim$7 Å and their dynamical correlation decays on a time scale of $\sim$3 ps, as found for density fluctuations in a recent study [PRL **106**, 037801 (2011)].

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